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Numerical Solution of Generalized IHCP by Discrete Mollification

C. E. MEJÍA*
Universidad Nacional de Colombia
Departamento de Matemáticas
Apartado Aéreo 3840, Medellín, Colombia
cemejia@perseus.unalmed.edu.co

D. A. MURIO†
Department of Mathematical Sciences
University of Cincinnati
Cincinnati, OH 45221-0025, U.S.A.
diego@dmurio.csm.uc.edu

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Abstract—A numerical space marching algorithm based on discrete mollification and automatic iterative filtering by Generalized Cross Validation is applied to the solution of a generalized one-dimensional inverse heat conduction problem. No information about the noise is assumed. With data temperature and heat flux functions measured at a discrete set of points on the boundary $x = 1$, $0 \leq t \leq 1$, the temperature and heat flux solution functions are approximately recovered in the unit square of the (x, t) plane, including its boundaries. Error bounds and numerical examples are provided.

Keywords—Ill-posed problems, IHCP, Parabolic equations, Marching schemes, Finite differences, Automatic filtering.

1. INTRODUCTION

Mollification has proven to be an appropriate method for smoothing noisy data and computing approximate solutions of ill-posed problems. In this paper we introduce a rigorous definition of discrete mollification and fully discuss its corresponding consistency and stability properties. The selection of the mollification parameter has been enhanced with the implementation of the Principle of Generalized Cross Validation. The new strategy is completely automatic and provides for the correct degree of smoothing of the mollified noisy data.

The main objective of the paper is the introduction of a numerical method for the solution of a generalized one-dimensional IHCP on the region $[0,1] \times [0,1]$ of the (x,t) plane when the data are given as noisy discrete versions of the temperature and heat flux functions at the active boundary $x = 1$ and for time values restricted to the interval $[0,1]$. The problem is solved on the entire region, *including its boundaries*, by combining a stable space marching finite difference scheme and mollification at each step. Rigorous stability analysis and associated error bounds are provided.

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The paper is organized as follows: discrete mollification and the usual related estimates are discussed in Section 2. Automatic numerical differentiation based on discrete mollification is presented in Section 3 and it is widely used in Section 4 where the generalized IHCP is investigated. Section 5 includes considerations on the implementation of the algorithm and numerical results.

2. MOLLIFICATION

The Mollification Method is a filtering procedure that is appropriate for the regularization of a variety of ill-posed problems. In this section we introduce the method and prove the main results.

2.1. Abstract Setting

Let $p > 0$, $\delta > 0$ and $A_p = (\int_{-p}^{p} \exp(-s^2)\,ds)^{-1}$. The δ-mollification of an integrable function is based on convolution with the kernel

$$\rho_{\delta,p}(t) = \begin{cases} A_p \delta^{-1} \exp\left(-\dfrac{t^2}{\delta^2}\right), & |t| < p\delta, \\ 0, & |t| \geq p\delta. \end{cases}$$

The δ-mollifier $\rho_{\delta,p}$ is a nonnegative $C^\infty(-p\delta, p\delta)$ function vanishing outside $(-p\delta, p\delta)$ and satisfying $\int_{-p\delta}^{p\delta} \rho_{\delta,p}(t)\,dt = 1$.

Let $I = [0,1]$ and $I_\delta = [p\delta, 1 - p\delta]$. The interval I_δ is nonempty whenever $p < 1/2\delta$. If f is integrable on I, we define its δ-mollification on I_δ by the convolution

$$J_\delta f(t) = \int_0^1 \rho_\delta(t-s) f(s)\,ds,$$

where the p-dependency on the kernel has been dropped for simplicity of notation.

The δ-mollification of an integrable function satisfies well-known consistency and stability estimates. (See, for instance, [1].) From now on, C will represent a generic constant independent of δ.

LEMMA 2.1. CONSISTENCY.

1. *If f is uniformly Lipschitz on I, with Lipschitz constant L, then there exists a constant C such that*
$$\|J_\delta f - f\|_{\infty, I_\delta} \leq C\delta.$$
2. *If $f \in C^2(I)$, then there exists a constant C such that*
$$\left\|(J_\delta f)' - f'\right\|_{\infty, I_\delta} \leq C\delta.$$

PROOF. We show the proof of the first assertion. Let $t \in I_\delta$. Then

$$\begin{aligned} |J_\delta f(t) - f(t)| &= \left| \int_0^1 \rho_\delta(t-s) f(s)\,ds - f(t) \right| \\ &\leq \int_{-p\delta}^{p\delta} \rho_\delta(s)\,|f(t-s) - f(t)|\,ds \\ &\leq L \int_{-p\delta}^{p\delta} \rho_\delta(s)\,|s|\,ds \\ &= L A_p \delta \int_0^{p^2} e^{-s}\,ds \\ &\leq L A_p \delta. \end{aligned}$$

LEMMA 2.2. STABILITY. *If f and f^ϵ are integrable on I and $\|f - f^\epsilon\|_{\infty,I} \le \epsilon$, then there exists a constant C such that*

$$\|J_\delta f - J_\delta f^\epsilon\|_{\infty,I_\delta} \le \epsilon \quad \text{and} \quad \left\|(J_\delta f)' - (J_\delta f^\epsilon)'\right\|_{\infty,I_\delta} \le C\frac{\epsilon}{\delta}.$$

PROOF. The second proof rests on the differentiability of the kernel ρ_δ on $(-p\delta, p\delta)$. Let $t \in I_\delta$.

$$\begin{aligned}
\left|(J_\delta f)'(t) - (J_\delta f^\epsilon)'(t)\right| &= \left|\frac{d}{dt}\left[\int_{t-p\delta}^{t+p\delta} \rho_\delta(t-s)\,(f(s) - f^\epsilon(s))\,ds\right]\right| \\
&= \Big|\rho_\delta(-p\delta)\,(f(t+p\delta) - f^\epsilon(t+p\delta)) \\
&\quad - \rho_\delta(p\delta)\,(f(t-p\delta) - f^\epsilon(t-p\delta)) \\
&\quad + \int_{t-p\delta}^{t+p\delta}\left(\frac{d}{dt}\rho_\delta(t-s)\right)(f(s) - f^\epsilon(s))\,ds\Big| \\
&\le 2A_p\frac{\epsilon}{\delta} + \epsilon\int_{t-p\delta}^{t+p\delta}\left|\frac{d}{dt}\rho_\delta(t-s)\right|,
\end{aligned}$$

and the last integral is easily estimated as follows:

$$\begin{aligned}
\epsilon\int_{t-p\delta}^{t+p\delta}\left|\frac{d}{dt}\rho_\delta(t-s)\right| ds &= A_p\frac{\epsilon}{\delta}\int_{t-p\delta}^{t+p\delta}\left|-\frac{2(t-s)}{\delta^2}\right|\exp\left(-\frac{(t-s)^2}{\delta^2}\right) ds \\
&= 2A_p\frac{\epsilon}{\delta}\int_0^{p^2} e^{-s}\,ds \\
&\le 2A_p\frac{\epsilon}{\delta}.
\end{aligned}$$

2.2. Discrete Mollification

In order to define the δ-mollification of a discrete function, we consider n different numbers on I, say $t_1, t_2, \dots, t_n$, satisfying $0 \le t_1 < t_2 < \cdots < t_{n-1} < t_n \le 1$ and define $\Delta t = \max_{1\le j\le n-1}|t_{j+1} - t_j|$. Furthermore, we set $s_0 = 0$, $s_n = 1$ and for $j = 1, 2, \dots, n-1$, $s_j = (1/2)(t_j + t_{j+1})$. Let $G = \{g_j\}_{j=1}^n$ be a discrete function defined on the set $K = \{t_1, t_2, \dots, t_n\}$. The discrete δ-mollification of G is defined as follows.

For every $t \in I_\delta$,

$$g_\delta(t) = \sum_{j=1}^n\left(\int_{s_{j-1}}^{s_j}\rho_\delta(t-s)\,ds\right) g_j.$$

Notice that $\sum_{j=1}^n(\int_{s_{j-1}}^{s_j}\rho_\delta(t-s)\,ds) = \int_{-p\delta}^{p\delta}\rho_\delta(s)\,ds = 1$.

The consistency estimates for the discrete δ-mollification are presented in the following lemma.

LEMMA 2.3. CONSISTENCY OF DISCRETE MOLLIFICATION.

1. *If g is uniformly Lipschitz on I, with Lipschitz constant L, then there exists a constant C such that*
$$\|g_\delta - g\|_{\infty,I_\delta} \le C(\delta + \Delta t),$$
where g_δ is the discrete δ-mollification of $G = \{g_j\}_{j=1}^n$, the discrete version of g, defined by $g_j = g(t_j)$.
2. *If $g \in C^2(I)$, then there exists a constant C such that*
$$\left\|(g_\delta)' - g'\right\|_{\infty,I_\delta} \le C\left(\delta + \frac{\Delta t}{\delta}\right).$$

PROOF. Let $t \in I_\delta$.

1. For the first part, we prove

$$\|J_\delta g - g_\delta\|_{\infty, I_\delta} \le L\Delta t.$$

We have

$$\begin{aligned} |J_\delta g(t) - g_\delta(t)| &\le \sum_{j=1}^{n} \int_{s_{j-1}}^{s_j} \rho_\delta(t-s)\, |g(s) - g(t_j)|\, ds \\ &\le L \sum_{j=1}^{n} \int_{s_{j-1}}^{s_j} \rho_\delta(t-s)\, |s - t_j|\, ds \\ &\le L\Delta t. \end{aligned}$$

Now, since $\|g_\delta - g\|_{\infty, I_\delta} \le \|J_\delta g - g_\delta\|_{\infty, I_\delta} + \|J_\delta g - g\|_{\infty, I_\delta}$, then the desired result is obtained by using Lemma 2.1, Part 1.

2. By triangle inequality, $\|(g_\delta)' - g'\|_{\infty, I_\delta} \le \|(J_\delta g)' - (g_\delta)'\|_{\infty, I_\delta} + \|(J_\delta g)' - g'\|_{\infty, I_\delta}$.

The second term was estimated in Lemma 2.1, Part 2. For the first one, let L be a uniform Lipschitz constant for g on I. We have

$$\begin{aligned} \left|(g_\delta)'(t) - (J_\delta g)'(t)\right| &= \left| \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \frac{d}{dt}\rho_\delta(t-s)\, ds \right) g(t_j) - \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \frac{d}{dt}\rho_\delta(t-s) g(s)\, ds \right) \right| \\ &\le \sum_{j=1}^{n} \int_{s_{j-1}}^{s_j} \left| \frac{d}{dt}\rho_\delta(t-s) \right| |g(t_j) - g(s)|\, ds \\ &\le L\Delta t \int_0^1 \left| \frac{d}{dt}\rho_\delta(t-s) \right| ds \\ &= L\Delta t \int_{t-p\delta}^{t+p\delta} \left| \frac{d}{dt}\rho_\delta(t-s) \right| ds \\ &\le 2LA_p \frac{\Delta t}{\delta}. \end{aligned}$$

In most applications, the only available data is a perturbed discrete version of g, denoted $G^\epsilon = \{g_j^\epsilon\}_{j=1}^n$, satisfying $\|G - G^\epsilon\|_{\infty, K} \le \epsilon$, where $G = \{g(t_j)\}_{j=1}^n$. The stability of the discrete δ-mollification is proved in the following lemma.

LEMMA 2.4. STABILITY OF DISCRETE MOLLIFICATION. *If the discrete functions G and G^ϵ satisfy $\|G - G^\epsilon\|_{\infty, K} \le \epsilon$, then*

$$\|g_\delta^\epsilon - g_\delta\|_{\infty, I_\delta} \le \epsilon \quad \text{and} \quad \left\|(g_\delta^\epsilon)' - (g_\delta)'\right\|_{\infty, I_\delta} \le 2A_p \frac{\epsilon}{\delta}.$$

PROOF. We prove the second assertion.

$$\begin{aligned} \left| \frac{d}{dt} g_\delta^\epsilon(t) - \frac{d}{dt} g_\delta(t) \right| &= \left| \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \frac{d}{dt}\rho_\delta(t-s)\, ds \right) g_j^\epsilon - \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \frac{d}{dt}\rho_\delta(t-s)\, ds \right) g_j \right| \\ &\le \sum_{j=1}^{n} \int_{s_{j-1}}^{s_j} \left| \frac{d}{dt}\rho_\delta(t-s) \right| \left| g_j^\epsilon - g_j \right| ds \\ &\le \epsilon \sum_{j=1}^{n} \int_{s_{j-1}}^{s_j} \left| \frac{d}{dt}\rho_\delta(t-s) \right| ds \\ &\le 2A_p \frac{\epsilon}{\delta}. \end{aligned}$$

The next theorem indicates that the δ-mollification of G^ϵ is a reasonable approximation of the function g.

THEOREM 2.5. CONVERGENCE OF DISCRETE MOLLIFICATION. *If g is uniformly Lipschitz on I, with Lipschitz constant L, and the discrete functions G and G^ϵ satisfy $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then there exists a constant C such that*

$$\|g_\delta^\epsilon - g\|_{\infty,I_\delta} \le C\,(\epsilon + \delta + \Delta t)\,.$$

PROOF. Triangle inequality yields

$$\|g_\delta^\epsilon - g\|_{\infty,I_\delta} \le \|g_\delta^\epsilon - g_\delta\|_{\infty,I_\delta} + \|g_\delta - g\|_{\infty,I_\delta}\,,$$

and the two terms on the right-hand side are estimated by Lemmas 2.4 and 2.3, Part 1, respectively.

NOTE. The corresponding *abstract* convergence statement readily follows: $\|g_\delta^\epsilon - g\|_{\infty,I_\delta}$ tends to zero as δ, ϵ and Δt tend to zero. The *numerical* convergence result establishes that the computed mollified function g_δ^ϵ converges to the mollified function $J_\delta g$. More precisely, we have Lemma 2.6.

LEMMA 2.6. NUMERICAL CONVERGENCE OF DISCRETE MOLLIFICATION. *If the discrete functions G and G^ϵ satisfy $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then there exists a constant C such that*

$$\|g_\delta^\epsilon - J_\delta g\|_{\infty,I_\delta} \le C\,(\epsilon + \Delta t)\,.$$

3. DIFFERENTIATION

This section discusses the main results on stable computation of numerical differentiation by the mollification method. The next section will show that mollified time differentiation is of great importance in the solution of a generalized IHCP.

THEOREM 3.1. CONVERGENCE. *If $g \in C^2(I)$ and $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then there exists a constant C such that*

$$\left\|\frac{d}{dt}g_\delta^\epsilon - \frac{d}{dt}g\right\|_{\infty,I_\delta} \le C\left(\delta + \frac{\epsilon}{\delta} + \frac{\Delta t}{\delta}\right).$$

PROOF. Triangle inequality yields

$$\left\|\frac{d}{dt}g_\delta^\epsilon - \frac{d}{dt}g\right\|_{\infty,I_\delta} \le \|(g_\delta^\epsilon)' - (g_\delta)'\|_{\infty,I_\delta} + \|(g_\delta)' - g'\|_{\infty,I_\delta}\,.$$

The final result follows from estimation of the two terms on the right-hand side by Lemmas 2.4 and 2.3, Part 2, respectively.

NOTE. The corresponding *abstract* convergence statement should prescribe a link between the parameters $\delta, \Delta t$ and ϵ as ϵ tends to zero. We could establish convergence of $\frac{d}{dt}g_\delta^\epsilon$ to $\frac{d}{dt}g$ by prescribing a rule of this type: $\Delta t = \epsilon$ and $\delta = \epsilon^{1/2}$. This is a consequence of the ill-posedness of numerical differentiation.

A *numerical* convergence statement should relate $(g_\delta^\epsilon)'$ with $(J_\delta g)'$, that is, the computed derivative with the derivative of the mollified version of g. It is presented in the following lemma and states that, for fixed δ, $\|\frac{d}{dt}g_\delta^\epsilon - \frac{d}{dt}J_\delta g\|_{\infty,I_\delta}$ tends to zero as $\epsilon \to 0$ and $\Delta t \to 0$.

LEMMA 3.2. NUMERICAL CONVERGENCE. *If g is uniformly Lipschitz on I, with Lipschitz constant L, and the discrete functions G and G^ϵ satisfy $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then there exists a constant C such that*

$$\left\|\frac{d}{dt}g_\delta^\epsilon - \frac{d}{dt}J_\delta g\right\|_{\infty,I_\delta} \le C\left(\frac{\epsilon}{\delta} + \frac{\Delta t}{\delta}\right).$$

PROOF. We omit the proof.

Assuming, from now on, that $|t_{j+1} - t_j| = \Delta t$ for all $j = 1, 2, \ldots, n-1$, computations are performed with a centered difference approximation of the mollified derivative $(g_\delta^\epsilon)'$, denoted $D_0(g_\delta^\epsilon)$. The next lemma shows the relationship between these terms over the interval $\widetilde{I_\delta} \equiv [p\delta + \Delta t, 1 - p\delta - \Delta t]$.

LEMMA 3.3. *There exists a constant C_δ, independent of Δt, such that*

$$\left\| D_0\left(g_\delta^\epsilon\right) - (g_\delta^\epsilon)' \right\|_{\infty, \widetilde{I_\delta}} \leq C_\delta \left(\Delta t\right)^2.$$

PROOF. The proof is a simple application of Taylor's theorem with the constant C_δ representing an upper bound, in magnitude, for higher order derivatives of ρ_δ.

COROLLARY 3.4. *If $g \in C^2(I)$ and $\|G - G^\epsilon\|_{\infty,K} \leq \epsilon$, then there exists a constant C_δ, depending on δ, such that*

$$\left\| D_0\left(g_\delta^\epsilon\right) - \frac{d}{dt} g \right\|_{\infty, \widetilde{I_\delta}} \leq C\left(\delta + \frac{\epsilon}{\delta} + \frac{\Delta t}{\delta}\right) + C_\delta (\Delta t)^2.$$

NOTE. An *abstract* convergence statement would require knowledge of the constant C_δ, in order to link the parameters in a suitable way. Instead, we present a *numerical* convergence statement that is a direct consequence of Lemmas 3.2 and 3.3. For fixed δ, it establishes convergence of $\|D_0(g_\delta^\epsilon) - \frac{d}{dt} J_\delta g\|_{\infty, \widetilde{I_\delta}}$ to zero as ϵ and Δt tend to zero.

LEMMA 3.5. NUMERICAL CONVERGENCE. *If g is uniformly Lipschitz on I, with Lipschitz constant L, and the discrete functions G and G^ϵ satisfy $\|G - G^\epsilon\|_{\infty,K} \leq \epsilon$, then there exist a constant C and a constant C_δ, depending on δ, such that*

$$\left\| D_0\left(g_\delta^\epsilon\right) - \frac{d}{dt} J_\delta g \right\|_{\infty, \widetilde{I_\delta}} \leq C\left(\frac{\epsilon}{\delta} + \frac{\Delta t}{\delta}\right) + C_\delta (\Delta t)^2.$$

We define a discrete mollified differentiation operator D_0^δ by the following rule: $D_0^\delta(G) = D_0(g_\delta)|_{K \cap \widetilde{I_\delta}}$, where g_δ is the discrete mollification of the discrete function G and $D_0(g_\delta)$ is restricted to the grid points in $K \cap \widetilde{I_\delta}$. The next theorem states that this operator is bounded.

THEOREM 3.6. *If G is a discrete function defined on K, then there exists a constant C such that*

$$\left\| D_0^\delta(G) \right\|_{\infty, K \cap \widetilde{I_\delta}} \leq \frac{C}{\delta} \left\| G \right\|_{\infty, K}.$$

PROOF. By definition and the mean value theorem, for $t \in K \cap \widetilde{I_\delta}$ we have

$$\begin{aligned}
|D_0 g_\delta(t)| &= \left| \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \frac{1}{2\Delta t} \left(\rho_\delta(t + \Delta t - s) - \rho_\delta(t - \Delta t - s)\right) ds \right) g_j \right| \\
&\leq \|G\|_{\infty,K} \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \frac{1}{2\Delta t} \left|\rho_\delta(t + \Delta t - s) - \rho_\delta(t - \Delta t - s)\right| ds \right) \\
&= \|G\|_{\infty,K} \int_{-p\delta-\Delta t}^{p\delta+\Delta t} \left| \frac{d}{dt} \rho_\delta(t - \Delta t + \mu) \right| dt,
\end{aligned}$$

where $0 \le \mu \le 2\Delta t$. A careful integration process gives the result in the following way:

$$\begin{aligned}\int_{-p\delta-\Delta t}^{p\delta+\Delta t}\left|\frac{d}{dt}\rho_\delta(t-\Delta t+\mu)\right| dt &= \int_{-p\delta-2\Delta t}^{p\delta}\left|\frac{d}{dt}\rho_\delta(t+\mu)\right| dt \\ &= \int_{-p\delta-2\Delta t+2\mu}^{p\delta+\mu}\left|\frac{d}{dt}\rho_\delta(t)\right| dt \\ &= \frac{A_p}{\delta}\int_{-p\delta-2\Delta t+2\mu}^{p\delta+\mu}\left|\frac{-2t}{\delta^2}\right| \exp\left(-\frac{t^2}{\delta^2}\right) dt \\ &= \frac{A_p}{\delta}\left\{\int_{-p\delta-2\Delta t+2\mu}^{0}\left(-\frac{2t}{\delta^2}\right)\exp\left(-\frac{t^2}{\delta^2}\right) dt\right. \\ &\quad \left.+\int_0^{p\delta+\mu}\frac{2t}{\delta^2}\exp\left(-\frac{t^2}{\delta^2}\right) dt\right\} \\ &= \frac{A_p}{\delta}\left\{1-\exp\left(-\frac{(-p\delta-2\Delta t+2\mu)^2}{\delta^2}\right)\right. \\ &\quad \left.-\exp\left(-\frac{(p\delta+\mu)^2}{\delta^2}\right)+1\right\} \\ &< 2\frac{A_p}{\delta}.\end{aligned}$$

4. GENERALIZED IHCP

4.1. Description of the Problem

We introduce a numerical method for the solution of the following one-dimensional generalized inverse heat conduction problem.

Find approximations for the temperature and heat flux functions, u and u_x, respectively, throughout the domain $[0,1] \times [0,1]$ of the (x,t) plane, from measured approximations of u and u_x in the time interval $[0,1]$ of the active boundary $x = 1$. More precisely, the functions u and u_x satisfy:

$$\begin{aligned} u_t &= u_{xx}, && 0<t<1, && 0<x<1, \\ u(1,t) &= \eta(t), && 0\le t\le 1, && \text{data}, \\ u_x(1,t) &= \sigma(t), && 0\le t\le 1, && \text{data}, \\ u(0,t) &= \alpha_*(t), && 0\le t\le 1, && \text{unknown}, \\ u_x(0,t) &= \beta_*(t), && 0\le t\le 1, && \text{unknown}, \\ u(x,0) &= \gamma_*(x), && 0\le x\le 1, && \text{unknown}, \\ u(x,1) &= \tau_*(x), && 0\le x\le 1, && \text{unknown}, \end{aligned} \tag{4.1}$$

where η and σ are not known exactly. The available data functions, η^ϵ and σ^ϵ, are measured approximations of η and σ, respectively, and they satisfy the estimates $\|\eta-\eta^\epsilon\|_{\infty,I} \le \epsilon$ and $\|\sigma-\sigma^\epsilon\|_{\infty,I} \le \epsilon$.

The numerical method consists on the implementation of the mollification method through a stable space marching finite difference scheme. Important features of this method are:

1. Automatic selection of regularization parameters according to the quality of the data. This is done through a combination of the mollification method and the principle of generalized cross validation (Section 5.1).
2. Implementation of an extension procedure that allows for calculation of mollifications and mollified derivatives for all $t \in [0,1]$ (Section 5.2).
3. The primary targets of the scheme are the heat flux u_x and the time derivative of the temperature, u_t. A standard procedure of mollified time differentiation is the key to solve the IHCP.

4.2. Regularized Problem

The first step is the regularization of problem (4.1) by the mollification method. The stabilized problem for $v = J_\delta u$ and $v_x = J_\delta u_x$ is:

$$\begin{aligned}
v_t &= v_{xx}, && 0 < t < 1, \quad 0 < x < 1, \\
v(1,t) &= J_\delta \eta(t), && 0 \le t \le 1, \\
v_x(1,t) &= J_\delta \sigma(t), && 0 \le t \le 1, \\
v(0,t) &= \alpha(t), && 0 \le t \le 1, \quad \text{unknown}, \\
v_x(0,t) &= \beta(t), && 0 \le t \le 1, \quad \text{unknown}, \\
v(x,0) &= \gamma(x), && 0 \le x \le 1, \quad \text{unknown}, \\
v(x,1) &= \tau(x), && 0 \le x \le 1, \quad \text{unknown}.
\end{aligned} \tag{4.2}$$

Let $h = \Delta x = 1/M$ and $k = \Delta t = 1/N$ be the parameters of the finite difference discretization. We denote by Q_j^n and W_j^n the discrete approximations of the mollified heat flux $v_x(jh, nk)$ and the mollified time derivative of temperature $v_t(jh, nk)$, respectively, obtained by the numerical method. At the j^{th} step, the algorithm produces Q_j^n and W_j^n for all $n = 1, 2, \ldots, N-1$.

The mollification parameter δ_i^j corresponds to the i^{th} mollification at the j^{th} step. There are three types of mollification parameters initially and one at each marching step, namely:

$i = 1$: Mollification of data temperature.

$i = 2$: Mollification of data heat flux.

$i = 3$: Mollified time differentiation of data temperature.

$i = 4$: Mollified time differentiation of heat flux.

4.3. The Algorithm

The algorithm for the method is as follows.

Input: Parameter p and grid sizes h and k.

Step 0:

1. Select δ_1^M and δ_2^M. Compute $\eta_{\delta_1^M}^\epsilon$ and $\sigma_{\delta_2^M}^\epsilon$ and extend them to the interval $[0, 1]$.
2. Select δ_3^M and perform mollified differentiation in time of $\eta_{\delta_1^M}^\epsilon$.
3. Select δ_4^M and perform mollified differentiation in time of $\sigma_{\delta_2^M}^\epsilon$.

Step 1: For $j = M, M-1, \ldots, 1$,

1. Compute $Q_{j-1}^n = Q_j^n - hW_j^n$, $n = 1, \ldots, N-1$.
2. Compute $W_{j-1}^n = W_j^n - hD_0^{\delta_4^j} Q_j^n$, $n = 1, \ldots, N-1$.
3. Select δ_4^{j-1} and perform mollified differentiation in time of Q_{j-1}^n.
4. Perform extension procedure to find Q_{j-1}^0 and Q_{j-1}^N.

Step 2: Use a quadrature formula to approximate:

$$\begin{aligned}
&v(jh, 0) \text{ from } Q_j^0, && j = 0, \ldots, M, \\
&v(jh, 1) \text{ from } Q_j^N, && j = 0, \ldots, M, \\
&v(0, nk) \text{ from } W_0^n, && n = 0, \ldots, N.
\end{aligned}$$

NOTE.

1. The algorithm does not require *a priori* knowledge of ϵ.

2. The differential equation $u_t = u_{xx}$ can be replaced by the more general model $u_t = (au_x)_x + f$, where a and f are known functions of (x,t). In this case, we set $P_j^n = a_j^n (u_x)_j^n$ and $R_j^n = (u_t)_j^n$. The numerical scheme becomes

$$\text{New } P_j^n = P_j^n - h\left(R_j^n - f_j^n\right),$$
$$\text{New } R_j^n = R_j^n - hD_0^{\delta^j}\left(\frac{P_j^n}{a_j^n}\right),$$

which is similar to the above scheme. This is an indication of the generality of the algorithm.

4.4. Analysis

The stability of the method is proved in the following theorem.

In what follows, we denote $|F_j| = \max_n |F_j^n|$ and C_δ represents a generic constant depending on the mollification parameters involved.

THEOREM 4.1. STABILITY OF THE ALGORITHM. *There exists a constant C such that*

$$\max\{|Q_0|,|W_0|\} \le \left(\exp\left(\frac{C}{\delta_4}\right)\right)\max\{|Q_M|,|W_M|\},$$

where $\delta_4 = \min_j \delta_4^j$.

PROOF. From the scheme we readily see that

$$\left|Q_{j-1}^n\right| \le \left|Q_j^n\right| + h\left|W_j^n\right| \le (1+h)\max\{|Q_j|,|W_j|\},$$

and

$$\left|W_{j-1}^n\right| \le \left|W_j^n\right| + h\left|D_0^{\delta_4^j}Q_j^n\right| \le \left|W_j^n\right| + h\left\|D_0^{\delta_4^j}\right\||Q_j|$$
$$\le \left(1+2hA_p\frac{1}{\delta_4}\right)\max\{|Qj|,|W_j|\}.$$

Thus,

$$|Q_{j-1}| \le (1+h)\max\{|Qj|,|W_j|\},$$

and

$$|W_{j-1}| \le \left(1+2hA_p\frac{1}{\delta_4}\right)\max\{|Qj|,|W_j|\},$$

which yields

$$\max\{|Q_{j-1}|,|W_{j-1}|\} \le (1+hM_\delta)\max\{|Qj|,|W_j|\},$$

where $M_\delta = \max\{1, 2A_p/\delta_4\}$.

The iteration of the last inequality leads us to

$$\max\{|Q_0|,|W_0|\} \le (1+hM_\delta)^M\max\{|Q_M|,|W_M|\}$$

and this implies

$$\max\{|Q_0|,|W_0|\} \le (\exp(M_\delta))\max\{|Q_M|,|W_M|\}.$$

The convergence of the numerical solution to the solution of the mollified problem (4.2) will be established next. We begin with the definition of the error functions

$$\Delta Q_j^n = \left(J_{\delta_2^j} u_x\right)_j^n - Q_j^n,$$
$$\Delta W_j^n = \left(\frac{\partial}{\partial t} J_{\delta_1^j} u\right)_j^n - W_j^n.$$

LEMMA 4.2.

1. *There exists a constant C_δ such that*

$$\left|\left(\frac{\partial}{\partial t} J_{\delta_2^j} u_x\right)_j^n - D_0^{\delta_4^j} Q_j^n\right| \le C_\delta (\Delta t)^2 + \frac{2A_p}{\delta_4^j} \left|\Delta Q_j^n\right|.$$

2. *There exists a constant C_δ such that*

$$\left|\left(\frac{\partial}{\partial t} J_{\delta_1^M} u\right)_M^n - \left(D_0 \left(J_{\delta_1^M} u^\epsilon\right)_{\delta_3^M}\right)_M^n\right| \le C_\delta (\Delta t)^2 + \frac{2A_p \epsilon}{\delta_3^M}.$$

PROOF. The proofs are consequences of Lemma 3.3 and Theorem 3.6. The first one is

$$\left|\left(\frac{\partial}{\partial t} J_{\delta_2^j} u_x\right)_j^n - D_0^{\delta_4^j} Q_j^n\right| = \left|\left(\frac{\partial}{\partial t} J_{\delta_2^j} u_x\right)_j^n - \left(D_0 \left(J_{\delta_2^j} u_x\right)_{\delta_4^j}\right)_j^n + \left(D_0 \left(J_{\delta_2^j} u_x\right)_{\delta_4^j}\right)_j^n - D_0^{\delta_4^j} Q_j^n\right|$$
$$\le C_\delta (\Delta t)^2 + \left\|D_0^{\delta_4^j}\right\|_{\infty, K \cap \tilde{I}_{\delta_4^j}} \left|\Delta Q_j^n\right|.$$

The initial errors ΔQ_M^n and ΔW_M^n are estimated in the following lemma.

LEMMA 4.3. *The initial errors ΔQ_M^n and ΔW_M^n satisfy the following estimates:*

1. *There exists a constant C, independent of δ, such that*

$$\left|\Delta Q_M\right| \le C \Delta t + \epsilon.$$

2. *There exist a constant C, independent of δ, and a constant C_δ, dependent on δ_3^M, such that*

$$\left|\Delta W_M\right| \le C_\delta (\Delta t)^2 + \left(\frac{2A_p}{\delta_3^M}\right)(\epsilon + C \Delta t).$$

PROOF. We present the second proof. It is based on Lemmas 4.2 and 2.3.

$$\left|\Delta W_M\right| = \max_n \left|\left(\frac{\partial}{\partial t} J_{\delta_1^M} u\right)_M^n - \left(D_0^{\delta_3^M} u_{\delta_1^M}^\epsilon\right)_M^n\right|$$
$$= \max_n \left|\left(\frac{\partial}{\partial t} J_{\delta_1^M} u\right)_M^n - \left(D_0^{\delta_3^M} J_{\delta_1^M} u^\epsilon\right)_M^n + \left(D_0^{\delta_3^M} J_{\delta_1^M} u^\epsilon\right)_M^n - \left(D_0^{\delta_3^M} u_{\delta_1^M}^\epsilon\right)_M^n\right|$$
$$\le C_\delta (\Delta t)^2 + \left(\frac{2A_p}{\delta_3^M}\right)(\epsilon + C \Delta t).$$

The error functions satisfy the following system of difference equations

$$\Delta Q_j^n = \Delta Q_{j+1}^n - h \Delta W_{j+1}^n + C_\delta h,$$
$$\Delta W_j^n = \Delta W_{j+1}^n - h \left[\left(\frac{\partial}{\partial t} J_{\delta_2^{j+1}} u_x\right)_{j+1}^n - D_0^{\delta_4^{j+1}} Q_{j+1}^n\right] + C_\delta h.$$

From Lemma 4.2 and writing $\delta_4 = \min_j \delta_4^j$, this system yields the inequalities

$$|\Delta Q_j| \le |\Delta Q_{j+1}| + h\,|\Delta W_{j+1}| + C_\delta h,$$
$$|\Delta W_j| \le |\Delta W_{j+1}| + \frac{2A_p}{\delta_4} h\,|\Delta Q_{j+1}| + C_\delta\left(h + \Delta t^2\right),$$

which in turn imply

$$|\Delta Q_j| \le (1 + C_\delta h)\max\left\{|\Delta Q_{j+1}|, |\Delta W_{j+1}|\right\},$$
$$|\Delta W_j| \le \left(1 + \frac{2A_p C_\delta}{\delta_4} h + C_\delta \Delta t^2\right)\max\left\{|\Delta Q_{j+1}|, |\Delta W_{j+1}|\right\}.$$

Thus, we have

$$\max\left\{|\Delta Q_j|, |\Delta W_j|\right\} \le \left(1 + hM_\delta + C_\delta \Delta t^2\right)\max\left\{|\Delta Q_{j+1}|, |\Delta W_{j+1}|\right\},$$

where $M_\delta = \max\{C_\delta, 2A_p C_\delta/\delta_4\}$.

Iteration of this inequality gives

$$\max\left\{|\Delta Q_0|, |\Delta W_0|\right\} \le \left(1 + hM_\delta + C_\delta \Delta t^2\right)^M \max\left\{|\Delta Q_M|, |\Delta W_M|\right\},$$

and this implies

$$\max\left\{|\Delta Q_0|, |\Delta W_0|\right\} \le \left(\exp\left(M_\delta + C_\delta \frac{\Delta t^2}{h}\right)\right)\max\left\{|\Delta Q_M|, |\Delta W_M|\right\}.$$

Consequently, if we fix the (δ_i^j)'s and impose the condition $\lim_{\Delta t \to 0, h \to 0}(\Delta t^2/h) = C$, Lemma 4.3 and the above considerations provide the proof of the following convergence theorem.

THEOREM 4.4. CONVERGENCE OF THE ALGORITHM. *If* $\lim_{\Delta t \to 0, h \to 0}(\Delta t^2/h) = C$, *then* $\max\{|\Delta Q_0|, |\Delta W_0|\}$ *tends to zero as* $\Delta t, h$ *and* ϵ *tend to zero.*

5. NUMERICAL IMPLEMENTATION

5.1. Selection of Regularization Parameters

Computation of $(g_\delta^\epsilon)_k$ can be viewed as

$$\sum_{i=1}^{n} [A_\delta]_{ki}\, g_i^\epsilon = \left(g_\delta^\epsilon\right)_k,$$

where

$$[A_\delta]_{ki} = \int_{s_{i-1}}^{s_i} \rho_\delta(t_k - s)\, ds,$$

and $G = \{g_i^\epsilon\}_{i=0}^N$ is the noisy data function. Since the noise in the data is not known, an appropriate mollification parameter, introducing the correct degree of smoothing, should be selected. Such a parameter is determined by the Principle of Generalized Cross Validation as the value of δ that minimizes the functional

$$\frac{\left(G^\epsilon\right)^\top \left(I^\top - A_\delta^\top\right)\left(I - A_\delta\right) G^\epsilon}{\text{Trace}\left[\left(I^\top - A_\delta^\top\right)\left(I - A_\delta\right)\right]}.$$

After computing g_δ^ϵ, the desired δ-minimizer is obtained by a Golden Section Search Procedure. Basic references on the subject are [2–4].

5.2. Extension of Data

Computation of $J_\delta(g)$ and g_δ throughout the time domain $I = [0,1]$ requires either the extension of g to a slightly bigger interval $I'_\delta = [-p\delta, 1+p\delta]$ or the consideration of g restricted to the subinterval $I_\delta = [p\delta, 1-p\delta]$. Our approach is the first one. We seek constant extensions g^* of g to the intervals $[-p\delta, 0]$ and $[1, 1+p\delta]$, satisfying the conditions

$$\|J_\delta(g^*) - g\|_{L^2[0,p\delta]} \text{ is minimum,}$$

and

$$\|J_\delta(g^*) - g\|_{L^2[1-p\delta,1]} \text{ is minimum.}$$

The unique solution to this optimization problem at the boundary $x = 1$ is given by

$$g^* = \frac{\int_{1-p\delta}^{1} \left[g(t) - \int_0^1 \rho_\delta(t-s)g(s)\,ds\right]\left[\int_1^{1+p\delta} \rho_\delta(t-s)\,ds\right] dt}{\int_{1-p\delta}^{1} \left[\int_1^{1+p\delta} \rho_\delta(t-s)\,ds\right]^2 dt}.$$

A similar result holds at the end point $t = 0$. A proof of these statements can be found in [5].

5.3. Numerical Results

The algorithm of the previous section has been thoroughly tested. In this section we present numerical results from two examples. In all cases, the discretization parameters are as follows: The number of space divisions is M and $\Delta x = h = 1/M$; the number of time divisions is N and $\Delta t = k = 1/N$; the maximum level of noise in the data function is ϵ; the mollification parameters are denoted δ if there is no confusion and, without loss of generality, we set $p = 3$. The value $p = 3$ is appropriate because the difference between ρ_δ for $p = 3$ and ρ_δ for $p > 3$ is not significant.

The use of average perturbation values ϵ is only necessary for the purpose of preparing the simulations. The filtering procedure introduced here automatically adapts the regularization parameters to the quality of the data.

Discretized measured approximations of the boundary data are simulated by adding random errors to the exact data functions. Specifically, for a boundary data function $\alpha(t)$, its discrete noisy version is

$$\alpha_n^\epsilon = \alpha(t_n) + \epsilon_n, \qquad n = 0, 1, \ldots, N,$$

where the (ϵ_n)'s are Gaussian random variables with variance $\sigma^2 = \epsilon^2$.

In order to test the stability and accuracy of the algorithm, we consider two examples and a selection of average noise perturbations ϵ, and space and time discretization parameters, h and k. The errors at the boundaries $x = 0$, $t = 0$ and $t = 1$ are measured by the weighted l^2-norms defined as follows.

Error in the heat flux at $x = 0$:

$$\left[\frac{1}{N}\sum_{n=1}^{N} |\beta_*(t_n) - Q_0^n|^2\right]^{1/2}.$$

Error in the temperature at $x = 0$:

$$\left[\frac{1}{N}\sum_{n=1}^{N} |\alpha_*(t_n) - U_0^n|^2\right]^{1/2},$$

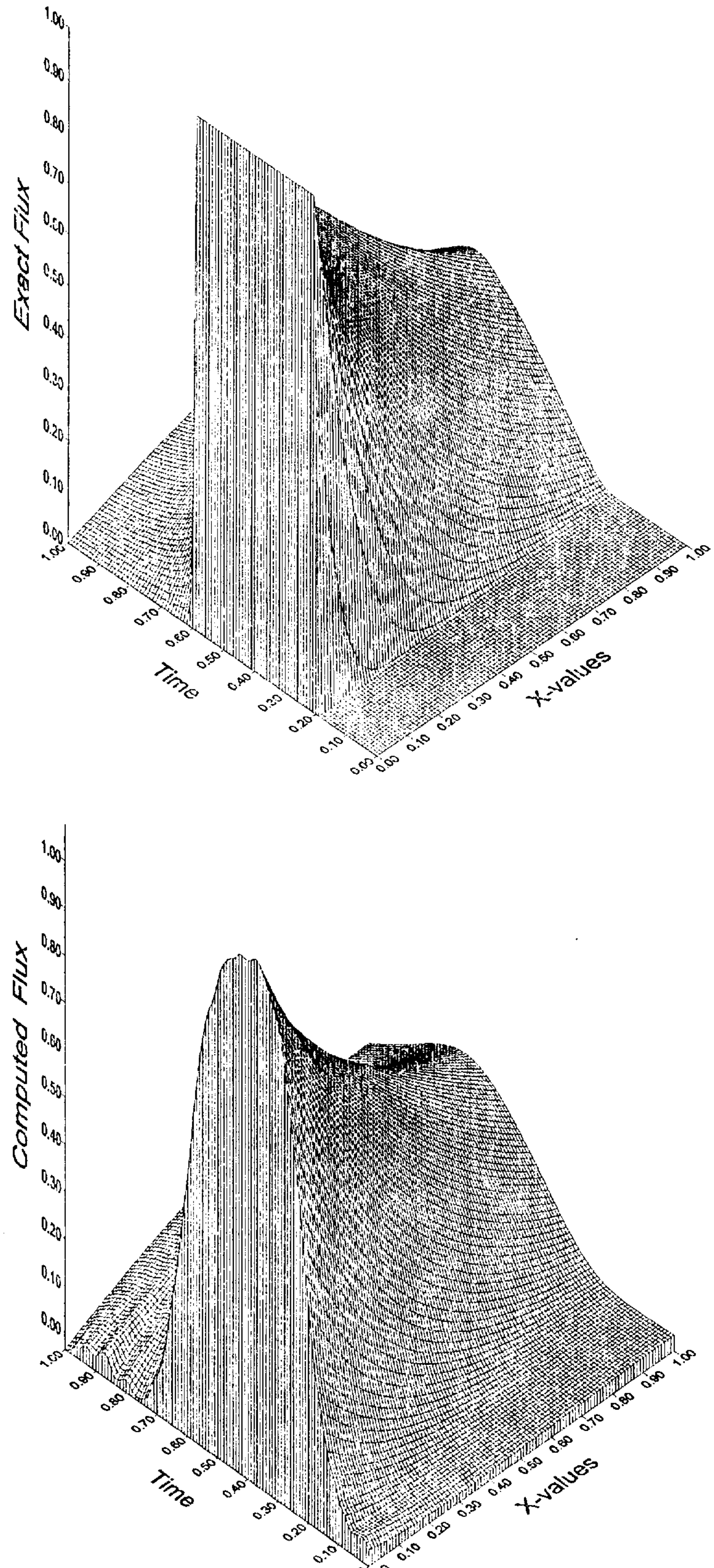

Figure 5.3.1. Problem 1. Exact and computed heat flux surfaces with parameters $p = 3$, $\Delta x = h = 1/100$, $\Delta t = k = 1/128$. Simulated noise level: $\epsilon = 0.005$.

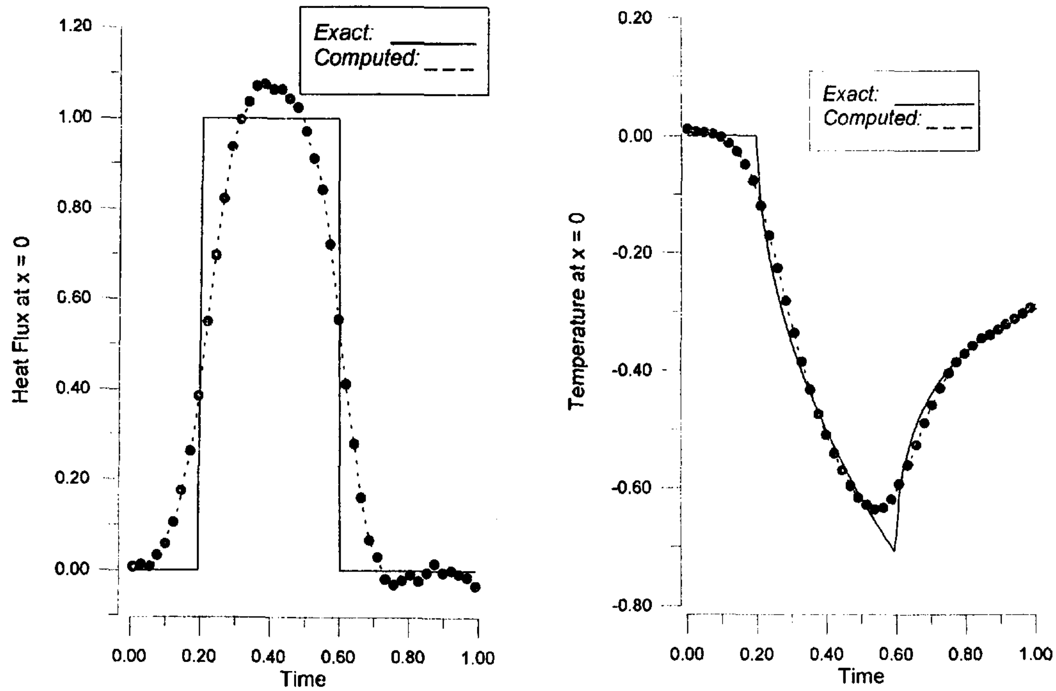

Figure 5.3.2. Problem 1. Exact and computed heat flux and temperature functions at $x = 0$ with parameters $p = 3$, $\Delta x = h = 1/100$, $\Delta t = k = 1/128$. Simulated noise level: $\epsilon = 0.005$.

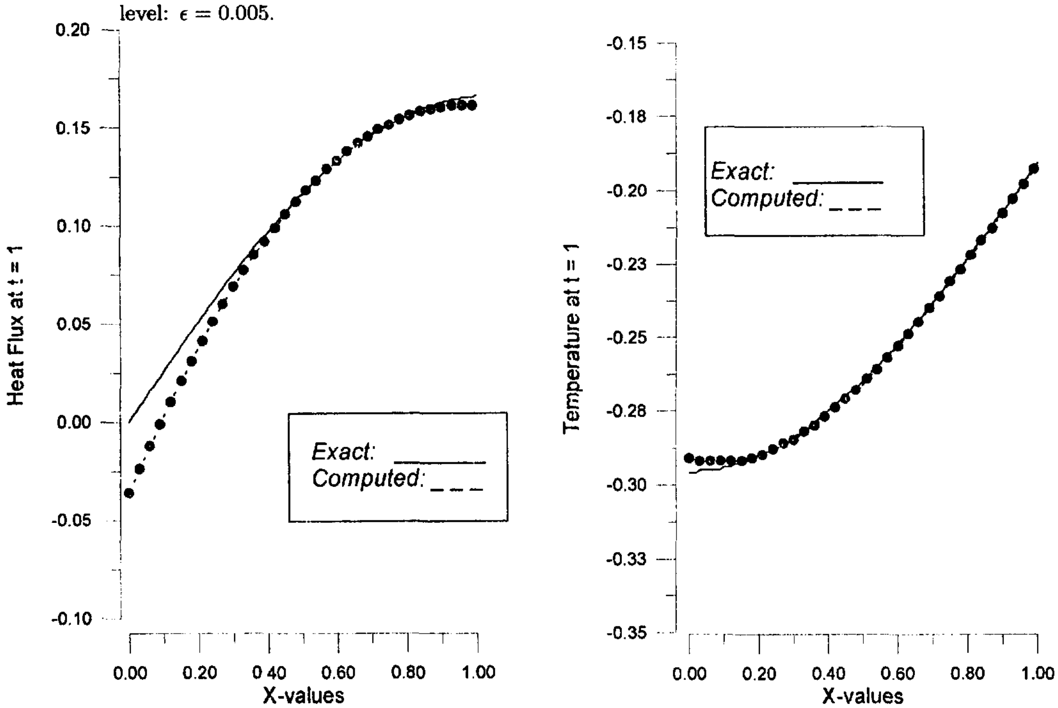

Figure 5.3.3. Problem 1. Exact and computed heat flux and temperature functions at $t = 1$ with parameters $p = 3$, $\Delta x = h = 1/100$, $\Delta t = k = 1/128$. Simulated noise level: $\epsilon = 0.005$.

where U_0^n is the approximate boundary temperature obtained from W_0^n by a quadrature rule. Similar formulations are utilized at the boundaries $t = 0$ and $t = 1$.

We recall that the maximum error norm estimates of Section 4 are also valid for the weighted l^2-norms since we always have

$$\left[\frac{1}{N}\sum_{n=1}^{N}|F_0^n|^2\right]^{1/2} \leq \max_n |F_0^n| .$$

All the tables were prepared with $\Delta t = k = 1/128$. No significant changes occur if we consider values of the time discretization parameter in the (tested) interval $[1/32, 1/256]$.

PROBLEM 1. This prototype example emphasizes the estimation of a transient unit step heat flux at $x = 0$ for $0.2 \le t \le 0.6$, from transient data measured at $x = 1$, $0 \le t \le 1$. The recovery of boundary conditions of this type constitutes a real challenge for any numerical algorithm. The mathematical description of the problem is given by

$$\begin{aligned} u_t &= u_{xx}, && 0 < x < 1, \quad 0 < t < 1, \\ u(1,t) &= f(t), && 0 \le t \le 1, \\ u_x(1,t) &= q(t), && 0 \le t \le 1, \end{aligned}$$

where

$$f(t) = \widetilde{f}(t - 0.2) - \widetilde{f}(t - 0.6),$$

with

$$\widetilde{f}(t) = \begin{cases} -2\sqrt{\dfrac{t}{\pi}} \exp \dfrac{-1}{4t} + erfc \dfrac{1}{2\sqrt{t}}, & 0 < t, \\ 0, & 0 \ge t, \end{cases}$$

and

$$q(t) = \widetilde{q}(t - 0.2) - \widetilde{q}(t - 0.6),$$

with

$$\widetilde{q}(t) = \begin{cases} erfc \dfrac{1}{\sqrt{t}}, & 0 < t, \\ 0, & 0 \ge t. \end{cases}$$

The corresponding boundary heat flux at $x = 0$ is given by

$$Q(t) = \begin{cases} 0, & 0 \le t \le 0.2, \\ 1, & 0.2 < t \le 0.6, \\ 0, & 0.6 < t \le 1. \end{cases}$$

Table 5.3.1. Problem 1. Errors at $x = 0$, with parameters $p = 3$, $\Delta t = k = 1/128$.

Simulated noise level: $\epsilon = 0.000$		
h	Temperature	Heat flux
1/16	0.0272	0.1654
1/32	0.0071	0.1035
1/100	0.0112	0.0742
1/128	0.0133	0.0761
1/200	0.0154	0.0825
1/400	0.0171	0.0940

Table 5.3.2. Problem 1. Errors at $x = 0$, with parameters $p = 3$, $\Delta t = k = 1/128$.

Simulated noise level: $\epsilon = 0.005$		
h	Temperature	Heat flux
1/16	0.0310	0.1714
1/32	0.0201	0.1438
1/100	0.0213	0.1365
1/128	0.0212	0.1372
1/200	0.0223	0.1382
1/400	0.0240	0.1421

Table 5.3.3. Problem 1. Errors at $x = 0$, with parameters $p = 3$, $\Delta t = k = 1/128$.

Simulated noise level: $\epsilon = 0.010$		
h	Temperature	Heat flux
1/16	0.0359	0.1813
1/32	0.0281	0.1625
1/100	0.0282	0.1633
1/128	0.0289	0.1620
1/200	0.0290	0.1618
1/400	0.0301	0.1621

Figures 5.3.1–5.3.3 give a clear qualitative indication of the excellent approximate solutions obtained with the method. Further verifications of stability and accuracy are provided by the combination of parameters that yields the data in Tables 5.3.1 to 5.3.3.

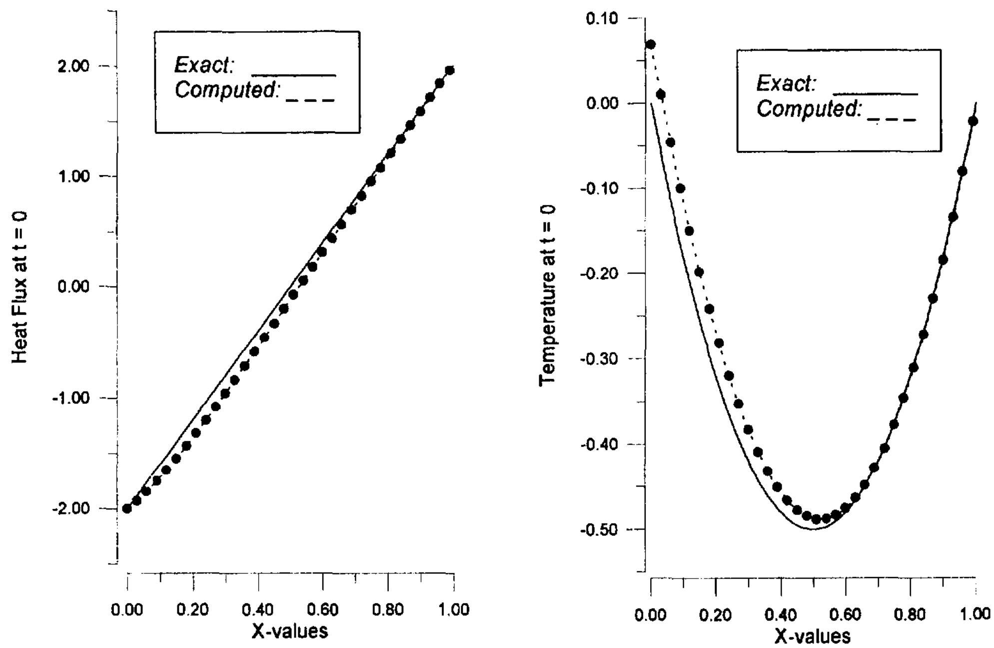

Figure 5.3.4. Problem 2. Exact and computed heat flux and temperature functions at $t = 0$ with parameters $p = 3$, $\Delta x = h = 1/100$, $\Delta t = k = 1/128$. Simulated noise level: $\epsilon = 0.005$.

PROBLEM 2. This example is designed to stress the behavior of the method when attempting to recover the "initial" and "final" time conditions at $t = 0$ and $t = 1$, respectively. To that effect, we consider the diffusion process

$$\begin{aligned} u_t &= u_{xx} + F(x,t), && 0 < x < 1, \quad 0 < t < 1, \\ u(1,t) &= f(t), && 0 \le t \le 1, \\ u_x(1,t) &= q(t), && 0 \le t \le 1, \end{aligned}$$

where

$$\begin{aligned} F(x,t) &= x(1-x) + 2(t-2), && 0 \le t \le 1, \quad 0 \le x \le 1, \\ f(t) &= 0, && 0 \le t \le 1, \end{aligned}$$

and

$$q(t) = 2(1-t^2), \qquad 0 \le t \le 1.$$

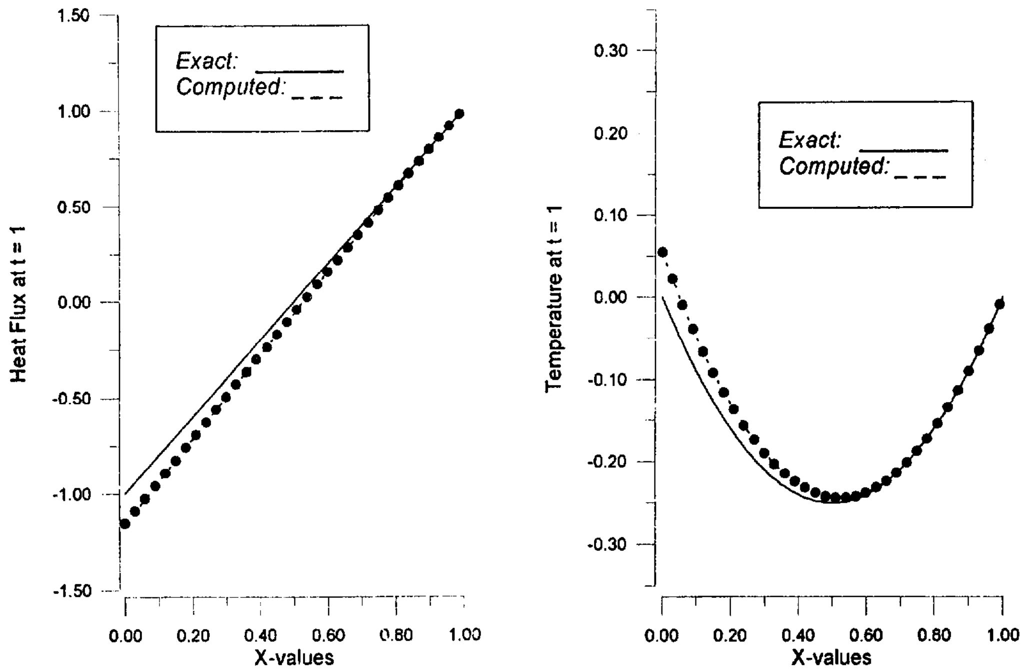

Figure 5.3.5. Problem 2. Exact and computed heat flux and temperature functions at $t = 1$ with parameters $p = 3$, $\Delta x = h = 1/100$, $\Delta t = k = 1/128$. Simulated noise level: $\epsilon = 0.005$.

Table 5.3.4. Problem 2. Errors at $t = 0$ and $t = 1$, with parameters $p = 3$, $\Delta t = k = 1/128$.

Simulated noise level: $\epsilon = 0.000$				
	Temp.	Temp.	Heat Flux	Heat Flux
h	$t = 0$	$t = 1$	$t = 0$	$t = 1$
1/16	0.0721	0.0362	0.0135	0.0321
1/32	0.0352	0.0181	0.0060	0.0058
1/100	0.0113	0.0101	0.0023	0.0100
1/128	0.0086	0.0073	0.0013	0.0161
1/200	0.0056	0.0051	0.0012	0.0152
1/400	0.0027	0.0039	0.0006	0.0134

Table 5.3.5. Problem 2. Errors at $t = 0$ and $t = 1$, with parameters $p = 3$, $\Delta t = k = 1/128$.

Simulated noise level: $\epsilon = 0.005$				
	Temp.	Temp.	Heat flux	Heat flux
h	$t = 0$	$t = 1$	$t = 0$	$t = 1$
1/16	0.0746	0.0525	0.0081	0.0547
1/32	0.0372	0.0355	0.0092	0.0589
1/100	0.0127	0.0244	0.0091	0.0618
1/128	0.0103	0.0233	0.0091	0.0619
1/200	0.0072	0.0217	0.0092	0.0616
1/400	0.0044	0.0200	0.0093	0.0603

The data and forcing term are such that the corresponding heat flux boundary functions at $t = 0$ and $t = 1$ are both quadratic in x, a challenging situation that eliminates the particular behaviors associated sometimes with the presence of monotone solutions.

Figures 5.3.4 and 5.3.5 show the excellent agreement between the computed and the exact temperature and heat flux functions at $t = 0$ and $t = 1$, obtained while marching from $x = 1$ to $x = 0$, under a moderate amount of noise level in the data ($\epsilon = 0.005$). Note that the actual temperature input is just the simulated discrete noise data function itself.

For Problem 2, Tables 5.3.4 to 5.3.6 further illustrate the stability properties and the practical accuracy of the method.

Table 5.3.6. Problem 2. Errors at $t = 0$ and $t = 1$, with parameters $p = 3$, $\Delta t = k = 1/128$.

Simulated noise level: $\epsilon = 0.010$				
	Temp.	Temp.	Heat Flux	Heat Flux
h	$t = 0$	$t = 1$	$t = 0$	$t = 1$
1/16	0.0395	0.0381	0.0089	0.0570
1/32	0.0364	0.0345	0.0088	0.0565
1/100	0.0119	0.0234	0.0084	0.0595
1/128	0.0097	0.0214	0.0086	0.0596
1/200	0.0064	0.0207	0.0083	0.0593
1/400	0.0037	0.0190	0.0084	0.0580

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